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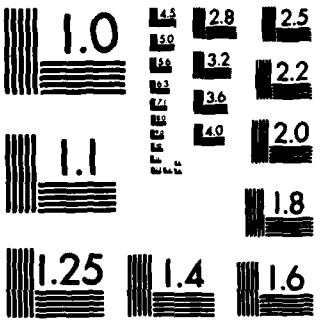

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18. SUPPLEMENTARY NOTES

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Gas-phase collision processes, chemiluminescence, laser fluorescence, alkaline earth atoms, oxidation reactions, dissociation energies, molecular energy transfer, spin-orbit states, open-shell molecules, semi-empirical potential energy surfaces.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A collaborative experimental and theoretical study both of the reactions of electronically excited alkaline earth atoms with molecular oxidants and of inelastic and reactive processes involving open-shell atoms and molecules has been carried out. The branching ratios for formation of ground and excited state products from the reactions of both ground state (^1S) and metastable electronically excited ($^3P^o$, ^1D, or ^3D) Mg, Ca, Sr, and Ba were determined by chemiluminescence and laser fluorescence measurements. These results were

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20. compared with adiabatic correlation predictions. It was also possible to set bounds on the CaO and MgO dissociation energies. A semi-empirical representation was developed for the description of the ion-pair (M^+O^-) potential energy surfaces for both alkali and alkaline earth atoms. A semi classical dipolar model was developed for the calculation of collisional interelectronic energy transfer rates between the low-lying $X\,^1\Sigma^+$, $a\,^3\Pi$, and $A\,^1\Pi$ states of CaO and used to interpret the observed pressure dependence of the Ca ($^3P^o$) + N_2O chemiluminescence spectrum. This model was also extended to energy transfer in MgO. Originator supplied keywords include:

An important general propensity rule in rotationally inelastic collisions of open-shell molecules has been discovered from an analysis of the appropriate quantum scattering equations, namely, that collisions preserving the internal reflection symmetry of the electronic wavefunction are favored. The electronic symmetry of Π state Λ-doublets has also been clarified, with implications for the interpretation of photodissociation and scattering experiments.

Collisional vibrational relaxation rates in the excited $A^2\Pi$ state of the CN radical were measured in a discharge flow apparatus. An optical pumping technique was developed for the study of collisions of individual spin-orbit states of Ca($4s4p\ ^3P_J^o$). A strong and unexpected variation of reactivity was observed both ground and excited state halide products from the Ca(^3P_J) + Cl_2 and Br_2 reactions. This effect was interpreted with the help of a quantum mechanical pseudo quenching dynamical model and an ab initio Ca Cl_2 potential energy surface. This optical pumping state-selection technique was also employed to measure cross sections for the structure-changing transitions of Ca($^3P^o$) with He, H_2, and D_2. Quantum mechanical close coupling calculations were carried out for Ca($^3P^o$) and Mg($^3P^o$) - He collisions with the help of pseudopotentials. An accurate ab initio Mg($^3P^o$) - He interaction potential was calculated and also employed in subsequent scattering calculations.

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ELECTRONICALLY EXCITED ALKALINE EARTH OXIDES: CHEMICAL PRODUCTION AND COLLISIONAL ENERGY TRANSFER PROCESSES

FINAL REPORT

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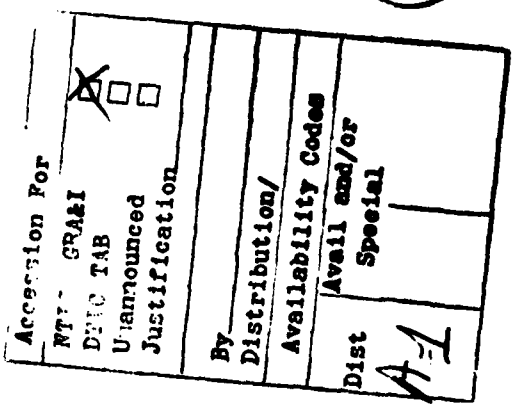

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STATEMENT OF THE PROBLEM STUDIED

One of the most exciting areas of chemical physics is the investigation of the dependence of kinetic processes on the internal electronic degrees of freedom of the species involved. New experimental advances, in particular the advent of tunable dye lasers, permit a far greater degree of both initial and final state resolution than has been hitherto possible. On the theoretical side, sophisticated angular momentum algebra, as well as fast scattering codes, have made accessible accurate quantum studies of inelastic collisions involving open-shell atoms and molecules. The study of these processes provides a direct probe of how the anisotropies of intermolecular potentials can effect changes in the electronic states of the collision partners, in other words, how the relative motion of atoms and molecules can be affected by and can affect the spin and orbital angular of their electrons. From a more practical viewpoint, a detailed understanding of the rates of collisional relaxation of electronic excited and open-shell atoms and molecules underlies our ability to model the temporal and spatial profiles of these species in combustion and chemical laser environments.

Over the past 6 years, supported by ARO grants DAAG29-78-G-0110 and DAAG29-81-K-0102, the two principal investigators of the present report have been involved in a collaborative experimental and theoretical study both of the reactions of electronically excited alkaline earth atoms with various molecular oxidants as well as of inelastic and reactive processes involving open-shell atoms and molecules.

SUMMARY OF THE MOST IMPORTANT RESULTS

1) The development of a new technique for the measurement of absolute yields for production of light emitting products. This method, applicable to reactions of electronically excited species, does not require any absolute photon intensity measurements.

2) Investigation of internal energy distributions and electronic branching ratios in reactions of ground and electronically ecited alkaline earth atoms with simple oxidants. Both chemiluminescence and laser-induced fluorescence detection were used to elucidate the branching ratios for production of ground and electronically excited products in the reactions of $Ca(^3P)$ and $Ca(^1D)$ with O_2, CO_2, and N_2O. These results were interpreted in terms of adiabatic correlation diagrams with the imposition of various dynamical constraints and were compared with the predictions of several statistical models. A dynamical interpretation was put forward which involved the well-known harpooning mechanism. The single-collision chemiluminescence from the reactions of $Sr(^1S)$ and metastable $Sr(^3P^\circ)$ and $Mg(^3P^\circ)$ with N_2O has been studied. The production of the nonemitting MgO x $^1\Sigma^+$ and $\underline{a}\ ^3\Pi$ states was also determined by laser fluorescence detection in $Mg(^3p^\circ)$ + N_2O and O_2. A model, based on orbital correlations, was developed for the N_2O reactions and was used to explain the large differences in the electronic state branching observed in the Ca and Sr reactions, as compared with Mg. Chemiluminescence from the reactions of ground-state $Ba(^1S)$ and metastable $Ba(^3D)$ with NO_2, N_2O, and O_3 was also studied under single-collision conditions. The dynamics of the Ba reactions were compared and contrasted with those of the lighter alkaline earth atoms.

3) New determination of dissociation energies of MgO and CaO. A careful study of near infrared chemiluminescence using photon counting techniques, was used to extract of a new, accurate value of the dissociation energy of the ground state ($X^1\Sigma^+$) of calcium oxide. Our result is in agreement with the thermochemically derived value but is significantly lower than the dissociation energy deduced in an earlier molecular beam study. Several Mg(^1S, $^3P°$) reactions were also examined in an attempt to resolve the disagreement between previous experimental determinations and a recent ab initio calculation of the MgO dissociation energy. Tentative support was obtained for the lower theoretical value.

4) The development of new semi-empirical representations of ion-pair ($M^+ - O_2^-$) potential surfaces. These species are key intermediates in reactive and/or inelastic collisions of alkali metals and alkaline earth atoms with molecular oxygen. We have developed a new semi-empirical form to describe these ion-pair intermediates, containing paramaters which can be calibrated from either matrix isolation experiments or ab initio studies.

5) Characterization of the production of both metastable states of atomic calcium (^3P and ^1D). A high temperature, electrically discharged, effusive oven, was developed for the production of electronically excited metastable states of alkaline earth atoms. Its operation with calcium was extensively studied and the conditions necessary for optimal stability and metastable conversion efficiency characterized. By variation of the atomic source conditions, we have shown how it is possible to vary substantially the $^3P°$ to ^1D population ratio in the beam.

6) The study of energy transfer in low-lying molecular excited states. The experimental investigation of the variation of the intensity and spectral distribution of the CaO chemiluminescence resulting from the Ca* + N_2O

reaction as a function of oxidant pressure has performed. Evidence has been obtained that nascent population is transferred by collisions from one or more non-radiating states into the radiating $A^1\Sigma^+$ state. Chemiluminescence was investigated up to pressures as high as 0.3 Torr. The yield of CaO $A^1\Sigma^+$ excited molecules was determined to increase significantly with N_2O pressure, indicative of facile collisional energy energy between nonemitting and emitting excited CaO* molecules. We also developed a simple theoretical model for these collisional processes, which can act to transfer population from nonradiating excited electronic states ($\underline{a}^3\pi$, $A'^1\pi$) into the radiating $A^1\Sigma^+$ state. In our model we postulate that collisional pumping between the $X^1\Sigma^+$, $A'^1\pi$, and $\underline{a}^3\pi$ state will occur efficiently through long-range dipole-dipole coupling involving polar oxidant molecules (N_2O, NO_2). This dipolar coupling will cause inter-electronic state transfer in the localized regions where mixing occurs due to non-Born-Oppenheimer perturbations.

Thermal rate constants for these collision induced transitions can be obtained as averages over bimolecular cross sections, which we are able to calculate within the microreversible Born approximation, developed in our research group. We used calculated rate constants to investigate population flow induced by collisions with N_2O and the pressure dependence of the (0,0) band in the CaO $A^1\Sigma^+ \rightarrow X^1\Sigma^+$ chemiluminescence spectrum. Subsequently, this dipolar model was extended to the ground $X^1\Sigma^+$ and low-lying $A^1\pi$ and $^3\pi_0$ states of MgO, in collisions with N_2O. New **ab initio** calculations of dipole moments in MgO were carried out, and the results used, within the first Born approximation, to determine cross sections for collision induced transitions between and among the $X^1\Sigma^+$, $A^1\pi$, and $\underline{a}^3\pi$ states. The probability for interstate transfer was found to be large in the neighborhood of the crossings between various rotational ladders.

A discharge flow apparatus has also been constructed and utilized for the investigation of collision processes in electronically excited CN. Vibrational relaxation in the $A^2\Pi$ state has been investigated through cw dye laser excitation in the $A^2\Pi - X^2\Sigma^+$ band system and observation of the emission from various vibrational levels as a function of pressure. Concurrently with the development of these experiments, we have made considerable progress in the formulation of the exact quantum theory of electronically inelastic collisions involving diatomic molecules in low-lying excited states. This work goes beyond the dipolar model described above.

7) Prediction of selection rules in rotationally inelastic collisions of open-shell diatomic molecules. Analysis of the quantum-mechanical equations which describe the collision of an atom with a molecule having non-zero spin and/or orbital angular momenta led to the conclusion that, independent of the interaction potential, transitions which preserve the internal reflection symmetry of the electronic wavefunction will be favored. This was the first theoretical prediction of such propensity rules, which had been observed in a few experiments. Our work encompassed both the formal analysis of collisions of molecules in $^{2,3}\Sigma$ and $^{2,3}\Pi$ electronic states, as well as the calculation of cross sections for the Ar + NO ($X^2\Pi$) system. In the case of collisions of $^3\Pi$ molecules we were able to show that collision-induced transitions between levels of differing e/f symmetry would be strictly forbidden within the $\Omega = 0$ spin-orbit manifold. In the case of $^3\Sigma$ molecules, we were able to extend our analysis to the general case of intermediate Hund's coupling. An outgrowth of this work was the clarification of the electronic symmetry properties of Π state Λ-doublets, with important implications for the interpretation of reactive scattering and photodissociation experiments.

8) Dependence on spin-orbit state of reactions of Ca(4s4p $^3P_J°$) with Cl_2, Br_2 and CH_3Cl. A novel optical pumping state selection technique has been developed to deplete selectively one of three spin-orbit states of Ca(4s4p $^3P_J°$). To select a particular level, the laser is tuned into coincidence with the appropriate 4s5s ^3S ← 4s4p $^3P_J°$ line near 610 nm. Since the excited state decays back to all the $^3P_J°$ levels, with sufficient laser power (found to be ~1mW/cm^2) the pumped level population can be removed and transferred to the other J levels. Detection of the resulting calcium halide products, in both ground and electronically excited states, indicated a strong and unexpected variation with initial spin-orbit state. This work represents the first direct measurement of reactions of individual spin-orbit states for an atom with small spin-orbit splitting. The variation in reactivity in the Ca(^3P) + Cl_2 reaction is J=2 > J=1 > J=0 for production of the $A^2\Pi$ and $B^2\Sigma^+$ CaCl excited states, but is reversed for production of the CaCl ground state ($X^2\Sigma^+$). We believe the opposite ordering of spin-orbit reactivity is due to selective removal of flux at the first ionic-covalent curve crossing. Interpretation of this spin-orbit effect has been guided by **ab initio** studies of $CaCl_2$ potential energy surfaces by D. R. Yarkony of The Johns Hopkins University. A dynamical model which includes the critical covalent-ionic interactions has been developed. This pseudoquenching model contains the important physical effects present in the reactive system (ionic-covalent curve crossing, interference between electrostatic and orbit-rotation coupling). Calculated pseudoquenching cross sections indicate that adiabatic correlation arguments can be used even in the limit of small spin-orbit splitting.

9) Investigation of intramultiplet transitions in collisions of ^3P alkaline earth atoms with He, H_2 and D_2. The optical pumping state selection technique

mentioned above has also been used to determine cross sections for spin-orbit changing transitions in collisions of Ca($4s4p\ ^3P_J°$) with helium and hydrogen, in a beam-static gas arrangement. In this method, a first dye laser selectively removes one spin-orbit level as described above, and the collisional population redistribution as a function of target gas pressure is probed by a second dye laser. The intramultiplet cross sections for collisions with H_2 and D_2 were found to be substantially larger than those observed with He.

The quantum close-coupling (CC) treatment of collisions of an atom in a ^3P state with a structureless target was developed and the formalism extended to collisions with H_2 and D_2. Actual calculations were carried out for collisions of Ca($4^3P°$) and Mg($3^3P°$) with He and Ar, based on pseudopotential descriptions of the interaction potentials. These represent the first fully quantum studies ever of intramultiplet transitions in alkaline earth atoms. Of the three independent $J \rightarrow J'$ cross sections, the $2 \rightarrow 1$ is predicted to be largest, in good qualitative agreement with the experimental cross sections. Recently the Mg-He pseudopotential results were contrasted with cross sections calculated from a sophisticated **ab initio** description of the relevant interatomic potentials. Particular emphasis was devoted to a fully relevant adiabatic interpretation of the magnitude and energy dependence of the intramultiplet cross sections.

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